

# Crystallography News

## British Crystallographic Association

Issue No. 141 June 2017  
ISSI 1467-2790



## Spring Meeting and Durham School Scenes

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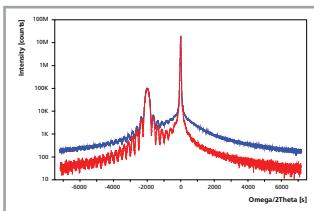
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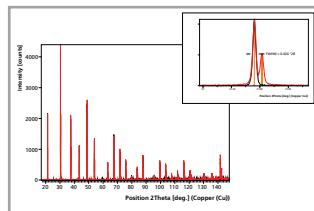
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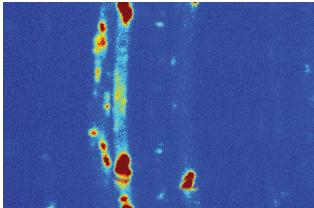
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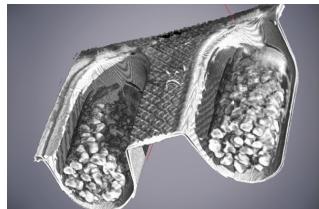
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CRYSTALLOGRAPHY NEWS is published quarterly (March, June, September and December) by the British Crystallographic Association, and printed by Bowmans, Leeds. Text should preferably be sent electronically as MSword documents (any version - .docx, .doc, .rtf or .txt files) or else on a PC disk. Diagrams and figures are most welcome, but please send them separately from text as .jpg, .gif, .tif, or .bmp files. Items may include technical articles, news about people (eg awards, honours, retirements etc), reports on past meetings of interest to crystallographers, notices of future meetings, historical reminiscences, letters to the editor, book, hardware or software reviews. Please ensure that items for inclusion in the September 2017 issue are sent to the Editor to arrive before 25 July 2017.

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Printed by Bowmans  
Westland Square, Westland Road, Leeds, LS11 5SS  
Tel: 0113 272 0088  
Web: [www.bowmans77.co.uk](http://www.bowmans77.co.uk)

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### This month's cover:

Spring Meeting scenes  
and Intensive School group,  
photos by Alice Clark,  
Horst Puschmann & CHS



# From the President



**AT** this time of year I'd like once again to reflect on an excellent Spring Meeting, held this year in Lancaster. I will be keen to see the formal feedback from those who attended, but anecdotally the feedback I received during the meeting was positive. As we look ahead to future meetings (more on this later) we are facing a challenge that fewer and fewer universities are making their accommodation available for conferences during the Easter break. Thus, we will need to rotate among a small number of venues or consider the possibility of moving away from university campuses.

The YCG satellite meeting continues to be a strong part of the overall Spring Meeting event and an excellent showcase for the diversity of science within the BCA. Congratulations also to the Early Career award winners: **Lauren Hatcher** (University of Bath), winner of the CCDC Chemical Crystallography Prize, **Atlanta Cook** (University of Edinburgh), winner of the BSG Prize, and **Phillip Maffetone** (University of Oxford) winner of the IG-YCG Prize.

I would like to congratulate **Stephen Moggach** on his election as Ordinary Member of BCA Council and thank **Amber Thompson**, whose term came to an end, for her contribution to the Council as an Ordinary Member over the past 6 years. As there were no nominations for the position of BCA Treasurer, Council have co-opted **Pamela Williams**, who has served as Treasurer for the past 5 years, to continue as Treasurer in the short term. We will seek to appoint a new Treasurer in the near future. I am grateful to Pamela not only for her years of service as Treasurer, but for her willingness to continue in the role in the interim.

The AGM held in Lancaster was very well attended and allowed us to have a very useful discussion of the two proposals brought by BCA Council that involved changes to the Statutes and By-Laws to enable a new process of nominations and voting for elections to BCA Council. Both motions passed overwhelmingly and will now be implemented. Full details will be provided on the BCA website, but are summarised below.

## **Proposal 1: BCA Council elections will be held ahead of the AGM with voting by electronic ballot.**

The anticipated advantages following implementation of the proposal are: (i) to maximise participation of the BCA membership in the elections; (ii) to ensure sufficient time at the AGM for discussion of reports and other matters; (iii) to allow smoother transition of Council members at the Spring Meeting.

The implementation of the proposal will involve: (i) a new nomination deadline, initially set to Sept 30th, approximately 6 months prior to the AGM; (ii) candidates providing a written statement in support of candidacy, a very brief CV and photograph to be published in December issue of Crystallography News; (iii) an electronic ballot open to the entire BCA membership during January.

## **Proposal 2: Establishment of a Nominating Committee**

Implementation involves (i) Appointment by Council of a Nominating Committee consisting of 5 members (Past-

President and one member from each of the BSG, CCG, IG and PCG groups). The Nominating Committee will aim to secure the nomination of two candidates for each Council vacancy.

It is important to note that no changes have been made to the current mechanism for nomination of candidates by two BCA members. This nomination process will continue alongside that involving the Nominating Committee, also using the **Sept 30th nomination deadline**. In the interests of fairness to all candidates, the mechanism by which candidates have been nominated will not be identified prior to elections. The inaugural BCA Nominating Committee has been appointed. Its members are: **Dave Keen** (BCA Past-President), **Elspeth Garman** (BSG), **Paul Raithby** (CCG), **Paul Fewster** (IG) and **Phil Lightfoot** (PCG). Nominations will be needed for the positions of President, Education & Outreach Officer and Ordinary member. I would like to encourage all BCA members to send suggestions for nominations to the new Nominating Committee or considering standing for election or making nominations themselves.

As the planning cycle for one BCA Spring Meeting ends another begins. The programme committee for the 2018 Spring Meeting at University of Warwick is in place (a full list of committee members is on the BCA website), and will be led by **Leo Brady** (University of Bristol). A preliminary meeting of the committee took place at the end of the Lancaster Spring Meeting and by the time this Newsletter is in print, the 2018 planning meeting will have been held at Warwick, symposia topics will be in place and invitations to plenary and keynote speakers will be going out. We are keen to encourage more input in terms of programme suggestions from the BCA membership via the programme committee members and I hope you have taken the opportunity to provide such input and will do so in future. Planning for the Autumn/Winter 1-day meetings organised by the BCA Groups is also getting underway.

Looking forward to the summer, the 24th triennial Congress of the IUCr will be held in Hyderabad, India. The UK is well represented among keynote lectures with **John Helliwell** (Manchester), **Nigel Unwin** (Cambridge), **Richard Henderson** (Cambridge) and **Neil Champness** (Nottingham) and from the UK scientific diaspora **Simon Billinge** (Columbia, NY).

I would like to conclude this column by congratulating scientists from the wider crystallographic community who have been recognised with the election to Fellowship of the Royal Society in 2017. Professor **Yvonne Jones** (University of Oxford) was elected based on her work in structural biology on “the molecular mechanisms by which cells signal to each other in the human body” (<https://royalsociety.org/people/yvonne-jones-13398/>). Professor **Sally Price** (UCL), who is a theoretical/computational chemist, was elected for her work in crystal structure prediction, which has contributed so much to our understanding of how and why organic molecules crystallise with the crystal structures that they do (<https://royalsociety.org/people/sarah-sallyprice13415/>).

Have a great summer.

**Lee Brammer**

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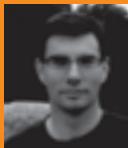


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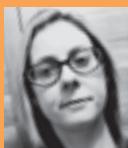
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Full committee details on the  
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**www.crystallography.org.uk**

# From the Editor



I WRITE this column soon after the very interesting BCA Spring Meeting. In this issue you will find several participants' descriptions of sessions that were of particular interest to them. I am deeply grateful to these authors for their completely voluntary contributions. I also give heartfelt thanks to Alice Clark for taking pictures at the conference dinner.

Most of my pictures of the ceilidh and some of the prize-giving illustrated what happens when you have excessively high anisotropic displacement parameters, while nearly all of Alice's are pin-sharp. In a normal year we have several bursary recipients who are required to write something for *Crystallography News*. However, it seems that this year all our members are so wealthy that they didn't apply for any bursaries; and therefore I am completely dependent on volunteers. As a hint for next year: if any of you become distressed millionaires facing the workhouse, do apply for a bursary to attend the 2018 Spring Meeting. It will be in the familiar comfortable surroundings of Warwick University.

This year marked the 30th anniversary of the Intensive Teaching School in X-ray Structure Analysis. As a Local Organiser of the first few Schools held at Aston University, I was delighted to be invited to the celebratory dinner at Durham and to meet some of the other staff from the first School. The evolution of the School's curriculum over the years documents the immense progress that has been made over the last 3 decades. An account of the latest School appears in this issue.

Two weeks before the BCA meeting I attended the annual meeting of the German Crystallographic Society (DGK). Although I shall present a write-up in the next issue, I can confirm now that his meeting had the usual DGK virtues: a friendly atmosphere, some very exciting plenary and keynote lectures about the latest advances in techniques and applications, a generally high standard of presentation in the official language (English) and generous amounts of excellent German beer and wine. In addition, we benefited from beautiful weather in Karlsruhe, which is located in a warm corner of southwest Germany famous for wine-growing. Although we had some chilly mornings, by early afternoon we enjoyed summer-like temperatures (around 293 K) under a blazing sun. My only disappointment was that I had a grand total of 2 people stopping to discuss my poster, which was in the area of structural systematics / crystal engineering. This may have happened because it was a poor poster; but when I displayed the same poster at the BCA meeting, I was kept talking beyond the official closing time of the poster session. My conclusion is that most German crystallographers are not very interested in these topics, while sizeable numbers of British (and American) crystallographers are.

On the subject of American crystallography, I am looking forward to the meeting of the American Crystallographic Association in New Orleans. Normally these meetings take

place in late July, but in IUCr Congress years they are moved to a southern city in late May (the 26th to 30th this year). One of my pleasant duties is to select a few General Interest posters that attract my attention and write about them in ACA RefleXions along with pictures of the proud presenters. Having been a university teacher for 38 years, the last thing I want to do is to apply some kind of marking system; but with it being clear that I'm just making an arbitrary choice of things that pique my interest, nobody worries about it. On the same trip to the USA one week before the ACA meeting I'll be attending my Class Reunion at Oberlin College in Ohio. At our previous reunion I was delighted to meet two of the professors who had taught me chemistry, then around 80 but still very fit. I hope I'll find them in similarly good condition this time.

Of course, the IUCr Congress in Hyderabad is coming ever closer. In commemoration of this event there is an Indian theme to the Puzzle Corner.

**John Helliwell** continues to dazzle us with his literary activity. One of his recent books has the title "*Perspectives in Crystallography*". Since it seems mainly destined for crystallographers' personal or research group libraries, I have reviewed it myself. John's other book, "*Skills for a Scientific Life*", has a much broader remit. Since readers may wish to consider purchasing it for a departmental or science faculty library, I have sought a complementary perspective and asked my eldest son to review it. Dr **Edward Schwalbe** is Senior Lecturer in Bioinformatics and Biostatistics at Northumbria University. One of his missions is to convince biological science students that statistics can be their friend.

In this issue I have the sad duty to print obituaries for two scientists who did much to safeguard crystallographers' efforts from error, viz. wrong absolute configuration or missed symmetry. **Howard Flack** benefited from top-quality crystallographic education in the UK, studying with **Kathleen Lonsdale** at University College London and then becoming a Research Assistant in Surface Physics in Cambridge. The combination of meeting a lovely Swiss girl and being offered a position in Geneva led Howard to spend the rest of his career based in Switzerland, though travelling widely. In the absence of careful measurements of Friedel pairs, absolute configuration had often been assigned by guesswork. Howard's derivation of the Flack parameter gave us reliable guidance. **Richard Marsh** did not have such personal connection with the UK, but his work did much to drive up the quality of structure determination here as elsewhere. Carefully surveying the crystallographic literature, he found distressingly many instances of missed symmetry and made crystallographers everywhere aware of this pitfall. The obituary written by colleagues at Caltech makes clear that, for all his zeal to eradicate errors, he was a valued friend and helpful mentor to his associates.

**Carl Schwalbe**



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## Answers to March Puzzle Corner



**EACH** of the three sets of clues will point you to the 9-letter name of a different element. The numbers from 1 to 9 correspond to letters. Different numbers could match the same letter. Deduce the correspondence for the words represented by the clues and enter the letters into the grid.

### Clues for Element 1:

- 12945 **GEMMA** is the name of a girl (who likes crystals?)  
 3512 **RAGE** is intense anger  
 867 **UNI** is short for an institution of higher learning

G	E	R	M	A	N	I	U	M
1	2	3	4	5	6	7	8	9

### Clues for Element 2:

- 234789 **ALLIUM** is the genus of plants including onion and garlic  
 13276 **PLAID** is Scottish fabric or a Welsh party  
 4591 **LAMP** is a light source

P	A	L	L	A	D	I	U	M
1	2	3	4	5	6	7	8	9

### Clues for Element 3:

- 2453 **OAST** is a house used for drying hops  
 6891 **SUMP** is a drainage receptacle  
 49765 **AMISS** is not quite right

P	O	T	A	S	S	I	U	M
1	2	3	4	5	6	7	8	9

# BCA Spring Meeting

THE 2017 BCA Spring Meeting took place at Lancaster University in conditions that were generally bright, but varying from breezy to downright blustery. The university is in the middle of a major reconstruction project affecting buildings along the main thoroughfare, called the Spine. Thanks to the designers' clever planning and liberal placement of signage, we still could take reasonably direct routes between our residences, the lecture theatres and the exhibition space. Two of the signs seemed to be worded with the BCA in mind and are reproduced here: one specifically for the PCG and one that seems to represent a particularly difficult macromolecular structure. Having half-promised the presence of ducks at the venue in my March "From the Editor" column, I was pleased to see a sizeable flock, including a mother duck followed around by a gaggle of charming ducklings.



As usual, the last evening of the meeting featured a delicious dinner, followed by a cheerful ceilidh. The main course was duck, although we believe it wasn't quite as local as it could have been – food miles rather than food yards.

In the following reports the named, plenary and prize lectures are highlighted. A selection of symposia will also be summarised.

## Carl Schwalbe

## Plenary Lectures

### The Parkin Lecture

The fourth session of the 2017 Young Crystallographers' Group Satellite Meeting began with the Parkin Lecture. Each year this lecture is delivered by a young crystallographer who has made a significant contribution to solving challenges within crystallography through outreach.

This year the lecture, entitled 'Listen to the Data', was given by **Briony Yorke** (Universität Hamburg). The lecture focused primarily on the use of data sonification as an interesting approach to interpreting data. For example, by converting a large data set into a waveform you can listen to, you are able to hear the patterns and anomalies within that data set. There are examples of sonification that are already in common use, notably Geiger counters which produce audible clicks when detecting ionizing radiation.

Briony went on to explain that this approach to data representation is an opportunity to engage a wider audience in crystallography, and indeed analysing data in general. Not only could this approach help us better understand our data by considering it from a different perspective, visually and audibly, but it also highlights the beauty and symmetry present in the subject.

## George Sackman University of Oxford

## The Lonsdale Lecture

As usual, the Lonsdale Lecture with its emphasis both on education and on cutting-edge research provided a bridge between the YCs' Satellite Meeting and the Main Meeting. **Kay Diederichs** from the University of Konstanz did exactly that, under the title "Towards a better understanding of (non-)isomorphism in macromolecular crystallography". He began by discussing "What is non-isomorphism". The narrow meaning is variation of cell parameters. The wider meaning is anything that systematically changes intensities from one crystal to another. Homogeneity is required if data are to be averaged, and agreement of cell parameters is a necessary but not a sufficient condition. Kay cited the study of hen egg white lysozyme, measured at 84.2% relative humidity and deposited in the PDB as 3aw6 and at 71.9% relative humidity as 3aw7. Even though the same authors collected data on the same apparatus at the same temperature, attempted merging of the data gave a high R(int). This is a clear case of systematic error. Other systematic errors attributable to the crystal include compositional and conformational inhomogeneity and radiation damage. The X-ray source, the detector and the data processing software can contribute further systematic errors. Random error is inevitably present due to the quantum nature of matter, both in the process of counting photons and as electronic noise. When is it safe to merge datasets? Datasets can be treated as vectors in n-dimensional space. The scalar product  $x_1 \cdot x_2$  defines a correlation coefficient  $cc_{12}$ . These pairwise correlation coefficients can be subjected to hierarchical cluster analysis.

**Carl Schwalbe**



## CCG Plenary

### *Transition metal coordination polyhedral: shape, spin and secondary bonding*

The CCG Plenary talk was given by **Santiago Alvarez** (Universitat de Barcelona), who discussed coordination shape of metal-ligand bonded complexes and the distortions that these undergo. He discussed the effect of normalising the distorted coordination geometry to form the ideal for each coordination number. This approach was applied to both low spin and high spin metal centres, in which the geometry does not change with mono-dentate ligands, but the normalisation does not correct bidentate ligands where the shape is distorted due to the fixed geometry of the ligand. The talk covered many ligands and the distorted shapes that they produce, resulting in a catalogue of distortion types which can help to predict distortions that will occur for a given metal spin state, coordination number and ligand type.

**James Walker**  
University of Oxford



## PCG Plenary

**Sharon Ashbrook** (University of St Andrews) gave this year's PCG plenary concerning the investigation of disorder and dynamics in solids using NMR crystallography; a technique which combines NMR, first principles DFT calculations and diffraction experiments. Sharon began with an overview of solid state NMR and the ways in which DFT calculations can aid in spectra assignment and prediction, as well as a method to verify NMR parameters and experiment feasibility. As a probe of local structure, NMR is sensitive to disorder and any present will give rise to additional resonances, line splitting and line broadening in the spectra. Sharon presented findings on AlPO STA-2 and  $\text{La}_2\text{Sn}_{2-x}\text{Ti}_x\text{O}_7$  systems in which numerous models were constructed and compared against NMR spectra to determine the nature of the disorder. Sharon's work enables once poorly characterised structures to be better elucidated and has numerous applications, such as the encapsulation of radioactive waste by ceramic materials.

**Madeline Corman**  
University of Oxford

## IG Plenary



Under the title "Crystallography for aerospace and nuclear sectors – an industrial perspective of the next decade" **David Rugg** described research done by Rolls-Royce. The failure rate on 50 MW gas turbines is only about 1 in  $10^8$ . To design and develop a new one with such impressive reliability costs £500 million to £1 billion. To anticipate and solve new problems requires science, often done in industrial / academic

partnership. Optimising the front end of turbines involves timescales from nanoseconds to years and fatigue cycles from 1 (e.g. a bird strike) to  $10^9$ . "Metals tend to lie to you." With billions of microcrystals a specimen may appear homogeneous, but at the crystal level the strength may vary by a factor of 3. Transmission electron microscopy of deformed cantilevers showed that "soft" grains underwent plastic deformation, forcing neighbours to take the stress. Micro-scale testing showed that smaller grains have much greater resistance to fatigue. On an atomic scale, the Al atoms in Ti-Al alloy were shown to prefer to be near other Al atoms. Rapidly heating a metal with a high-power laser just before XFEL diffraction measurements yields information about materials at high strain rates.

**Carl Schwalbe**

## Joint IG-CCG session on Phase Transitions

**Quanshun Luo** (Sheffield Hallam University) began the session with "Applications of quantitative X-ray diffraction in advanced materials research". This presentation discussed a multiple Gaussian peak-fitting technique which is used to resolve overlapping powder diffraction peaks. Using this quantitative technique crystallographic parameters for different phases in multiphase samples can be determined.

This technique was illustrated with two examples. The first was to measure the lattice mismatch between matrix and precipitate phases in a Nimonic 263 superalloy. The second was to resolve the overlapping diffraction peaks of lath and plate martensites co-existing in a hardened medium carbon ultrahigh strength steel.

The second presentation stayed in Sheffield. With the title "Liquid exfoliation of functionalised layered metal-organic frameworks to nanosheets" **James Foster** (University of Sheffield) looked at phase transitions in very different materials, metal-organic nanosheets. Two-dimensional metal-organic frameworks were designed to aid exfoliation of layers into nanosheets. Ultrasound on these frameworks in solution forms nanosheets. Different phases of these nanosheets are formed depending on the solvent used. Scanning Electron Microscopy and Atomic Force Microscopy can be used to image these nanosheets.

Next, **Alex Cousen** (University of Bath) described "preparation, characterisation and preferential crystallisation of enantiomeric multi-component materials (MCM): the case of naproxen and 2-aminopyridine". Enantiomerically pure active pharmaceutical ingredients are desired by the pharmaceutical industry. They can be made by enantioselective synthesis with expensive catalysts or separated by expensive large-scale chromatography. Crystallisation may provide a better method. Crystal growth from a racemic mixture gives a racemic phase most commonly, a solid solution occasionally, but sometimes a conglomerate phase of separated enantiomers. Naproxen forms such a racemic phase. However, with 2-aminopyridine charge transfer occurs, and now crystals with (S)-naproxen have different morphology than those with (RS).

The final presentation of this session, given by **Željko Skoko** (University of Zagreb, Croatia), was entitled "One step closer



(L-R) Kathi Edkins, Durham University (now Queen's Belfast University), Alex Cousen, Bath University, Jonathan Foster, Sheffield University, Željko Skoko, University of Zagreb, Croatia, Quanshun Luo, Sheffield Hallam University, Tony Bell, Sheffield Hallam University

to solving a mystery - structural and theoretical study of the thermosalient phenomenon". He told us about some fascinating materials that have some very energetic phase transitions. In the thermosalient effect the energy of the phase transitions is sufficient to cause "jumping crystals!"

This lecture presented results on a combined powder diffraction and theoretical study of this effect in N'-2-propylidene-4-hydrobenzohydrazide. In these phase transitions the driving force for this effect seems to be immense negative thermal expansion.

**Tony Bell**  
Sheffield Hallam University

**Katharina Edkins**  
Durham University (now Queen's University Belfast)

**Alex Cousen**  
University of Bath



## The Bragg Lecture

**Mike Glazer** (University of Oxford) gave the prestigious Bragg Lecture on "The wondrous world of perovskites". These materials, which make up about 38% of the volume of the Earth, have the general formula  $ABX_3$ , where A and B are cations and X is an anion. Examples are  $\text{CaTiO}_3$  and  $\text{BaTiO}_3$ . The paradigm structure is simple, a cube with A in the centre plus B at the corners and X halfway along the edges. However, numerous variations are possible, which can lead to very interesting properties, including (last year) photovoltaic properties. Barium-doped  $\text{La}_2\text{CuO}_4$  was the first high-temperature superconductor. A cation can move off a high symmetry site, or an atom can be lost entirely. Octahedra can be tilted or distorted, and these effects can be explained by considering the ionic radii of cations. Tilting squeezes the A cation. Perovskites can be useful in the form of crystals, but also ceramics and thin films on a substrate. The pyroelectric effect in certain perovskites was first noted by Theophrastus for tourmaline. Pyroelectric thermal sensor arrays have valuable applications such as sensing people occupying a smoke-filled room or moving through a security barrier. The piezoelectric effect was discovered in 1880 and is used in igniters where a hammer strikes a crystal or ceramic to generate a spark. The reverse effect, where an electric field causes motion, is used in quartz crystal watches and also generated the sound waves used in World War II sonar.

Mike also gave the Bragg Lecture at the Royal Institution, where it was recorded. It is viewable at  
<https://www.youtube.com/watch?v=v9bMEUr2I4>  
or <http://tinyurl.com/nykch2k>

with questions at  
<https://www.youtube.com/watch?v=WsPBB6azzX4>  
or <http://tinyurl.com/mk5btfp>

**Carl Schwalbe**

## BSG Plenary

The final plenary lecture was given by **Erhard Hohenester** (Imperial College London) on "Structural biology of cell adhesion to laminin". Laminins are large glycoproteins which, polymerising at the cell surface, interact with keratin and other molecules to form basement membrane. Duchenne muscular dystrophy is caused by breakage of links to laminin leading to membrane damage. Inadequate repair results in fibrosis. Dystroglycan is a vital laminin receptor on muscle cells which must be glycosylated with a unique sugar (making it requires  $\approx 15$  enzymes, so it must be very important!). Failure of glycosylation leads to severe dystrophy. Binding of  $\alpha$ -dystroglycan to laminin requires  $\text{Ca}^{+2}$ . Attempts to soak laminin crystals with 1mM oligosaccharide cracked the crystals. Crystals slowly fed over 2 weeks survived, but the oligosaccharide was disordered across a symmetry centre. NMR titration of saccharide and laminin gave good data but requires lots of protein. Surface plasmon resonance is more economical. Binding of integrin by laminin requires the E8 fragment, and a mini-E8 fragment of  $\alpha$ ,  $\beta$  and  $\gamma$  chains with just the last 50 residues is still biologically active. Although this structure dissociated when held at pH 4.5 in an attempt to grow crystals, methylating the lysine residues led to good stable crystals. The structure resembles a ladle with a coiled coil of  $\alpha$ ,  $\beta$  and  $\gamma$  chains forming the handle.



**Carl Schwalbe**



Lauren Hatcher (R) with Andrew Maloney

## Prize Lectures

### CCDC-CCG Prize Lecture

#### Exciting molecules

Prize-winner **Lauren Hatcher** (University of Bath) described her progression into the photococrystallography of solid state linkage isomers. Concentrating on the conversion of nitro to nitrito complexes, she showed that rearrangements were accompanied by changes in bulk properties such as colour and refractive index that might be used for data storage. She has endeavoured to maximise photo-conversion by using bulky, chelating ancillary fragments that dominate the packing and create a "reaction cavity". An example is  $\text{Ni}(\text{Et}_4\text{dien})(\text{NO}_2)_2$ , which gives a nitrito product metastable at  $< 150\text{K}$ . Below this temperature one can collect a high-quality X-ray dataset on the unreacted crystal, then irradiate *in situ* by LED ring switched off when conversion is complete, and take a new data set on the photo-activated crystal. Up to  $170\text{K}$  one can carry out a pseudo-steady-state experiment, collecting data under continuous illumination. The nitro complex diminishes, nitrito increases, but an exo-nitrito product also forms. Goals for further research are to get greater conversion within a specified timeframe, increase the operating temperature and control the switching speed. Using heavier transition elements increases the upper temperature limit for metastability but decreases the efficiency of conversion and increases the switching time.

### BSG Early Career Prize

**Atlanta Cook** (University of Edinburgh) described her research into Tsr1, which acts as a molecular gatekeeper in the eukaryotic ribosome. In 1 minute yeast makes  $\approx 2000$  ribosomes. Ribosome biogenesis is costly, involving  $>350$  biogenesis factors, many of which are energy-requiring enzymes. To avoid wasting resources on malformed products, there are 3 quality-control steps. Immature 40S particles travel to the cytoplasm with specific biogenesis factors. The maturation check includes compatibility with 60S particles. The role of Tsr1 and when it is removed from pre-40S particles are subjects for research. Full length Tsr1 does not crystallize. With its loop 2 removed, it gives poor crystals. However, phasing was difficult. Molecular replacement failed, SeMet incorporation made the crystallization fail, Au, Hg and Pt derivatives did not work. Eventually,  $\text{Ta}_6\text{Br}_{12}$  made a useful heavy atom derivative, at least up to  $6 \text{ \AA}$ , and enabled the location of S sites. Single wavelength anomalous dispersion at  $1.77 \text{ \AA}$  for S enabled phase extension. Tsr1 was found to have a degenerated active site and a highly conserved positively charged back surface. It can be fitted into pre-40S particles.



Atlanta Cook (L) with Angela Cresswell (Rigaku)

## IG-YCG Prize

**Phillip Maffetone** (University of Oxford) told us about "Protein structure determination by Bayesian reverse Monte Carlo". Crystallizing a protein, particularly a membrane protein (1) is difficult and (2) may change its conformation. In the absence of a suitable crystal, the pair distribution function (PDF) provides useful conformational information. However, the PDF only provides a 1-dimensional map which needs to be augmented with other information to yield a 3-dimensional model. In fact, we do have a great deal of prior knowledge. From the sequence we can extract bond distances and angles. The Ramachandran distribution provides a wealth of information about  $\phi$  and  $\psi$  torsion angles. NMR chemical shifts are available from measurements in solution, and further information about  $\phi$  and  $\psi$  can be obtained by machine learning. By using this prior knowledge in a Bayesian approach it becomes possible to select the realistic solutions from the multitude of solutions produced by Monte Carlo calculations. Tests on melittin (taking 1 hour) and PDB entries 1LQ7 and 1PRB (taking 2 days) showed promise.

### Carl Schwalbe



Phillip Maffetone (R) with Tony Bell (Sheffield Hallam University)

application based on X-ray powder diffraction data: modelling of structural disorder in layered double hydroxides (LDHs). LDHs have the general formula  $[M^{2+}_{(1-x)}N^{3+}_x(OH)_2]^+[X^{n-(x/n)}]^- \cdot yH_2O$ , where M is a divalent metal, N is a trivalent metal and X is a charge-compensating anion located between positively charged layers. Such structures are liable to stacking faults. The DISCUS package enables the simulation of powder patterns for LDHs with variation in probability of interlayer shifts, 3D layer consistency and water content.

**Andrew Maloney** (CCDC) discussed what we can learn from solid form landscapes. As well as an answer to the question "which form has the lowest energy", information about properties is needed for drug product design. The morphology of a crystal can be conveniently represented by the ratios of dimensions of a bounding box, small:medium and medium:large. Mechanical properties arise from structure. The existence of slip planes facilitates tabletting. An algorithm can find the most efficient path through a simplified version of a structure, calculate the Miller plane it most closely follows and evaluate its rugosity. It would be useful to predict other properties, notably melting point and solubility.

**Doris Braun** (University of Innsbruck) addressed a fascinating conundrum. Brucine and strychnine have very similar chemical structures that feature hydrogen bond acceptor groups but no hydrogen bond donor groups, yet they differ radically in their diversity of crystal forms. For brucine 23 solid forms are known: 2 anhydrides, 4 hydrates, 16 solvates and an amorphous phase. Strychnine, on the other hand, has only one anhydrous form and two solvates. By calculation of crystal energy landscapes and analysis of packing in the known crystal structures Doris was able to explain these findings. Brucine hydrate A is non-stoichiometric and has water in channels, leading to isomorphism of hydrate and dehydrate and no hysteresis. The hydrogen bonding in brucine hydrates B and C involves water, leading to collapse on dehydration and a mixture of hydrates upon rehydration. Crystal structure prediction for strychnine gives a single clear minimum. Lattice energy calculations can be used to compare the stability of hydrates and anhydrides.

### Carl Schwalbe



(L-R) Andrew Maloney, Colin Seaton, Doris Braun, Wojciech Sławiński, Anthony Reilly, Krešo Bučar

## Selected Symposia

### Computational Approaches

**Colin Seaton** (University of Bradford) began the session with an overview of optimisation algorithms under the title "Replicate, divide, mutate, survive: applying differential evolution optimisation to crystals". Optimisation is a key method in science and engineering. Newtonian methods use derivatives, which may be difficult to calculate. Population-based methods avoid this requirement. Differential evolution represents trial solutions as real valued vectors. By recombination and mutation combined into a single step, child solutions are developed; the better one of parent and child is retained. An important application is to solve structures from X-ray powder diffraction data.

**Wojciech Sławiński** (STFC ISIS Facility) introduced another

## Chemical Insights from Charge Density

**Simon Parsons** (University of Edinburgh) opened this session with his keynote lecture on “The role of electron density in structure interpretation”. He began by summarising a much-used interpretation of atom-atom contact distances: if they are short, relative to the sum of van der Waals radii, the interaction is strong and stabilising; but if they are long, they can be neglected. This idea can be very misleading. Atoms can be forced together by other interactions, van der Waals radii are not sharp cut-offs, and widely used compilations of van der Waals radii like the one by Bondi are based on a limited set of very old data. “To understand phase stability, we must work in Joules not Å”. The PIXEL program [Dunitz & Gavezzotti (2005) *Angew Chem.*, **44**, 1766–1787] has liberated us from viewing intermolecular interactions solely as a collection of atom-atom contacts. It calculates coulombic, polarization, dispersion, and repulsion energies from the electron density of molecular clusters. To obtain the electron density, one plucks out one molecule from the asymmetric unit, calculates its electron density (Gaussian with B3LYP is good) and populates the unit cell with other blocks by using the space group symmetry. The pixel-pixel interactions are then worked out. Results agree well with those from the higher-level Symmetry-Adapted Perturbation Theory (SAPT). As an example of a phase change,  $\gamma$ -glycine changes to  $\epsilon$ -glycine at a pressure of 2–4 GPa. The  $\epsilon$  form is more efficiently packed, but full interaction maps for  $\gamma$ -glycine place carboxyl O atoms at expected sites while in  $\epsilon$  they are displaced.

Next, **Lucy Mapp** (University of Southampton) discussed “Understanding pharmaceutical co-crystal properties via charge density”. As an example, propyphenazone (which has a central ring with two nitrogen atoms and a carbonyl group but otherwise only aliphatic and aromatic substituents) crystallizes with co-formers bearing COOH, OH or both. From charge density results on such co-crystals Lucy found the critical points and bond paths and compared atomic charges to density at bond critical points. She could evaluate the significance of C=O interactions versus others (the COOH dimer looks stronger). Melting points correlate directly to the sum of interaction energies.

**Clare Stubbs** (University of Bath) showed how systematic manipulation of orbital interactions could tune the chemical properties of Pt(II) pincers. These are square planar complexes in which three Pt coordination sites are occupied by N, C and N atoms of a 2,6-dipyridylbenzene chelating ligand. The strong field keeps the antibonding  $d_{x^2-y^2}$  orbital unpopulated. The planar complexes tend to form 1-dimensional stacks with close Pt-Pt interactions. Spectroscopic properties can be tuned by the choice of ligand at the 4th coordination site (substituted acetylidene groups in this work) and substituent at the 4'-position of the phenyl ring. Computational, spectroscopic and crystallographic studies explain the changes in emission profiles.

The importance of longer-range interactions was underscored by **Claire Wilson** in her presentation on “Exploring secondary bonding in neutral Ge(II) complexes”. Such complexes with neutral N, P or As ligands and Cl, Br or I counter ions have variable coordination numbers, making computational modelling and crystal structure prediction very difficult. Experimental research is required to elucidate the interplay of weak secondary interactions. Charge density studies on  $\text{GeCl}_2(2,2'\text{-bipyridine})$  and  $\text{GeCl}_2(1,10\text{-phenanthroline})$  yield

bond path profiles showing electron density concentrated near the electronegative atom. Variable pressure structure determinations on these complexes show a difference of  $\approx 0.8$  Å between Ge-Cl1 and Ge-Cl2 distances at ambient pressure which disappears at 81 kbar.

## Carl Schwalbe



(L-R) Claire Wilson, Hazel Sparkes, Clare Stubbs, Simon Parsons, Lucy Mapp, Graham Tizzard

## Complementary Techniques

### Using NMR and first-principles calculation to understand disorder in molecular organic solids

The keynote talk of the complementary technique session was given by **Paul Hodgkinson** (Durham University). The use of NMR combined with first order calculation can be used to complement an incomplete single crystal X-ray diffraction analysis when studying disorder within molecular organic solids. Paul discussed NMR techniques as a way of analysing hydrogen bonds using variable temperature  ${}^2\text{H}$  relaxation times to determine how dynamic the hydrogen within the bond is. He went on to describe how computational NMR methods can accurately predict the experimental spectra and can be used to complement them, allowing for a greater understanding of the types of disorder occurring within molecules through methods other than X-ray diffraction.

**James Walker**  
University of Oxford

## Multi-Component Crystals

**Krešo Bučar** started this session off with “Engineering molecular crystals: backbreaking, yet gratifying”. He presented results on co-crystals of xanthines and benzoic acid, some of which confounded efforts to predict them. Co-crystals in the CSD of derivatives of theophylline and benzoic acid form synthons A, B and C with A and B equally frequent while C only occurs with multiple-carboxylic acids. With a fluorinated benzoic acid theophylline formed synthon A at UCL but synthon B in Cambridge. When the researchers exchanged

their chemicals, A still formed at UCL and B in Cambridge! The solvent may have an effect too. With a tetrafluorinated derivative, A formed in acetonitrile but B in nitromethane. Although a crystal energy landscape calculated for caffeine and benzoic acid predicted that a co-crystal could form, initial experiments failed to produce one. Addition of a seed with structure similar to that of the most stable predicted form led to co-crystals, and now caffeine plus benzoic acid always give co-crystals.

**Katharina Edkins** discussed "Substituent influence on self-assembly of pharmaceutical drug compounds". Her first model compound was 2,4-dihydroxybenzoic acid. As a test of added bulk, the 5-bromo and 3,5-dibromo derivatives were also crystallized. The profusion of polymorphs, hydrates and solvates suggests that the molecules are not "happy" in the crystalline state. A carboxylic acid dimer is formed by the parent compound, lost with one Br but restored with two. Her second model compound was triphenylimidazole, para-substituted on one benzene ring with Cl, Br or I. Crystals grown from acetonitrile have solvent in channels lined by Cl atoms, but with Br there is disorder. From methanol the Br and I derivatives behave similarly.

**Nicholas Blagden** told us about "Crystal growth considerations for crystal engineering". With crystals of di-leucine as an example he pointed out the need for a phase diagram and the importance of kinetics. Viewing crystal growth as a lock and key process highlights the impact of solvents and the importance of nucleation. Small dipeptides crystallize so as to associate the stronger acid with the best acceptor, and likewise the second strongest acid and acceptor. Since peptide synthesis often ends with trifluoroacetic acid (TFA) treatment, the strong TFA may go into the final crystal.

**Charlie McMonagle** looked at "Gas uptake within fullerene stabilised phthalocyanine nanoporous molecular crystals". A frequent problem with nanoporous molecular crystals is inefficient packing with clathrated solvent that leads to collapse if it is removed. However, combining a metal-containing phthalocyanine derivative with a C<sub>60</sub> fullerene produces co-crystals that retain their structure when heated, boiled in aqueous acid or base, or subjected to high pressure. The stability resembles that of MOFs, but there is a free metal site. With a Co<sup>2+</sup> phthalocyanine co-crystal after evacuation to remove solvent, CO or O<sub>2</sub> are efficiently but reversibly bound at pressures well below 1 atm. The C<sub>60</sub> fullerene appears to be tumbling, but a "rugby ball" C<sub>70</sub> has a preferred direction.

### Carl Schwalbe



(L-R) Gareth Lloyd, Charlie McMonagle, Krešo Bučar, Katharina Edkins, Hayley Green, Nicholas Blagden

# XRF and XRD Meetings – 2017



RSC | Advancing the  
Chemical Sciences

Atomic Spectroscopy Group  
Analytical Division, RSC

## 1. JOINT BCA/RSC XRF MEETING 14th June 2017 University of Leicester

More details and registration at: <https://sites.google.com/site/bcaxrf/meetings/14-june-2017>

## 2. BCA IG XRD Meeting 15th June 2017 at the same venue.

More details and registration at: <https://sites.google.com/site/bcaxrf/meetings/15-june-2017>

09:30 Registration, Coffee and Exhibition. Meeting closes at 17:00

Registration is now open but will close at 23:59 on Thursday 9th June.

**Fees:** **BOTH DAYS** £126 or £63 concessions.  
**ONE DAY** £84 or £42 concessions.

**CALL for papers – We are actively seeking speakers for both days – see meeting pages for details.** Talks combining XRF and XRD would be of particular interest. Contact any member of the committee if you are interested.

**Speakers on 15th June will include:-** Tony Bell (Sheffield Hallam University) – *How can XRF help with X-ray Powder Diffraction?*

A limited number of **FREE STUDENT PLACES** are available on both days. To apply please E-mail David Beveridge (XRF Chair) with your name, E-mail address and Institution for details. **NOTE: THE STANDARD REGISTRATION FORM DOES NOT SUPPORT FREE PLACES AND STUDENTS USING IT WILL BE CHARGED CONCESSION FEES.**

This meeting offers a great chance to discuss your requirements with major equipment suppliers in the exhibition.

# Prizes Awarded at BCA 2017

## BSG Prizes



1. **BSG07** *Structural Studies on deamidase toxins*  
**Amirul Adli bin Abd Aziz** (University of Sheffield).
2. **BSG02** *Structural studies of proteins in Lambda phage*  
**Naer Al-Kaabawi** (University of Sheffield).

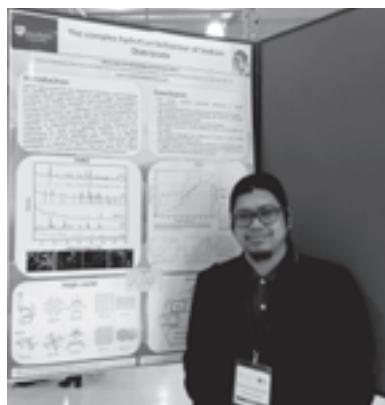
Matthew Conroy (PDBe) presenting the prizes to:  
**Amirul Adli bin Abd Aziz** (Far left) and **Naer Al-Kaabawi** (Far right)

## CCG Prizes



1. **CCG09** *Co-crystal or salt? Studying partial proton transfer in a series of molecular materials*  
**Mr James Walker**  
(University of Oxford).
2. **CCG24** *The complex hydration behaviour of sodium diatrizoate*  
**Mr Mohd Nadzri Bin Mohd Najib**  
(University of Durham).

The prize was presented by  
Stephen Moggach, CCG Chair



3. **CCG11** *Measuring and controlling dissolution rates of pharmaceutical materials by co-crystal formation*  
**Ms Laura Fenwick**  
(University of Oxford).

The prize was presented by  
Stephen Moggach, CCG Chair

## PCG Prizes



- PCG Prize PCG07**  
*Thermal processing of interstellar silicate analogues*  
**Anna Herlihy**  
(Diamond Light Source).

The prize was presented by  
Paul O'Meara, PANalytical



- Solid State Prize PCG08**  
*Ice-like disorder and diffuse scattering in Cd(CN)<sub>2</sub>*  
**Chloe Coates**  
(University of Oxford).

The prize was presented by  
Emma McCabe



(Left) **Paulo Lucaioli** (University of Lincoln) receiving YCG Flash Poster Presentation prize

The prize was presented by  
Sam Horrell, YCG chair

# Exhibitors at BCA 2017

Thank you to all exhibitors at **BCA Spring Meeting 2017**



1. Formulatrix
2. Scientific & Medical Products Ltd.
3. Rigaku Oxford Diffraction
4. PANalytical
5. Stoe
6. Oxford Cryosystems
7. Cambridge Crystallographic Data Centre
8. Bruker
9. Douglas Instruments
10. Cambridge Reactor Design
11. Incoatec

# BCA/CCG Intensive Teaching School

Photograph courtesy of Dr Horst Puschmann, Olexsys



## 16<sup>th</sup> BCA/CCG Intensive Teaching School in X-Ray Structure Analysis

25<sup>th</sup> March - 2<sup>nd</sup> April 2017, Trevelyan College, Durham, UK

**THE** 16th BCA/CCG Intensive Teaching School in X-ray Structure Analysis took place in Durham from the 25th March – 2nd April 2017. The school brings together students from a variety of countries, with different academic backgrounds and a range of crystallographic experience creating an interesting and friendly environment for meeting new people and learning. The 16th course was no exception being attended by 80 students who are studying or working in 16 different countries: the UK, Poland, Italy, Malta, Switzerland, Finland, Ireland, Brazil, Malaysia, Chile, Croatia, Germany, India, Uruguay, Saudi Arabia and Singapore. The majority of the students attending were PhD students with a small number of PDRA's and academic/industrial researchers all keen to learn more about crystallography. The national and international reputation of the school for providing a good basis in crystallography meant that we were once again heavily oversubscribed.

The course runs biennially and has evolved into its current format as a result of student and staff feedback as well as developments in equipment or methodologies which have also influenced the material covered. The course consists of a mixture of lectures and tutorials during which tutor groups work together to tackle a series of problems; each group consists of 8 students and a tutor who acts as a first port of call to help the students during the week. This year we

welcomed two new tutors, Dr **Andrew Cairns** and Dr **Nick Funnell**. The lectures and tutorials were held in the Sir James Knott Hall at Trevelyan College, which is an ideal space for the school allowing a quick switch between formal lecture presentations and tutorial work with minimal disruption. While the accommodation and meals, which were of a high standard, were provided less than a 5 minute walk away in Collingwood College.

During the 7-day course the students were once again guided through the various aspects of crystallography following on from an introductory session (Professor **William Clegg**). Lectures were given in the following order: Maths (Dr **Lukas Palatinus**), Symmetry (Professor William Clegg and Dr **Stephen Moggach**), Data Collection (Dr **Helena Shepherd**), Fourier Synthesis and Patterson (Professor William Clegg and Dr Stephen Moggach), Charge Flipping and Direct Methods (Dr Lukas Palatinus), Parameterisation and Least Squares (Professor **Simon Parsons**), Refinement (Professor **Richard Cooper**), Derivation of Results and Twinning (Professor Simon Parsons). Each of the main sessions consist of a combination of lectures to introduce topics and tutorial exercises designed to help the students improve their understanding of the material. In addition, optional presentations on Superspace (Dr Lukas Palatinus) and Synchrotrons and Neutrons (Dr **Mark Warren** and Dr **Mark Senn**) were given and well received with essentially full attendance.

As is traditional at the school, apart from the Maths lecture on the first evening, the evening activities are designed to be more relaxed and provide a chance for the students to mix with each other through a combination of educational and fun activities. This year's course was no exception with activities including a bar quiz (Professor Richard Cooper), useful tips on crystallisation (Dr **Dmitry Yufit**), a talk on databases focusing on the CSD and associated software (Dr **Peter Wood**) and student presentations (Dr **Katharina Edkins** and Dr **Helena Shepherd**). As usual the student presentations were of a very high standard and provided a very amusing evening in which each tutor group presented a short play on a scientific topic in a certain theme both of which had been randomly chosen earlier in the week e.g. neutron diffraction as a musical or crystallisation in the style of a game show. The presentations were designed to be educational as well as entertaining and our elite panel of judges, the lecturers, were very impressed by all of the entries.

The conference dinner on the Saturday evening provided a chance to thank all of the contributors to the school, the local staff, organisers, lectures, tutors and students for helping to make it a very successful school. As this year's school marked 30 years since the courses started at Aston University in 1987, we were delighted to have four of the founding members present at the conference dinner Dr **David Watkin**, Professor **Carl Schwalbe**, Professor **Bill Clegg** and Professor **Judith Howard** whose enthusiasm and initial setting of the ethos have helped to make the school what it is today. Both Bill, as a lecturer, and Judith, as an organiser, have been associated with the school throughout the 30 years which is some achievement! To mark this Bill revived an old tradition and put together a school song describing events from the week in an

amusing fashion, which he sang for us at the conference dinner to the tune of a Gilbert and Sullivan piece. However, Bill has decided to step-down from teaching at the school after this year's course and we will all miss his Escher T-shirts, wildlife pictures and jokes at future schools! Most of all though we will miss Bill's huge enthusiasm for teaching and communicating crystallography which along with his clear explanations and patience have benefited many students on the course over its 30 year history. Therefore, I would like say a huge THANK YOU to Bill for his enormous contributions to the school on behalf of myself, the school staff and all of the students who have attended the courses.

Following on from the success of the Olex2 workshop introduced for the first time after the previous school as a response to student feedback, Dr **Horst Puschmann** and Dr **Oleg Dolomanov** (OlexSys) ran another hands-on optional one day Olex2 workshop on Sunday the 2nd of April. This provided the 50 registered participants with a chance to use Olex2 to apply structure solution and refinement concepts that they had learnt on the course to both test structures and their own data and was very well received.

I would like to finish by saying thank you to all of the sponsors for this year's school, which were Diamond, IUCr, ECA, CCG, ICG, Oxford Cryosystems, Bruker, Rigaku Oxford Diffraction, CCDC and Pfizer. Without the financial support from these organisation we would not have been able to help as many students attend the school or run it so successfully and we are very grateful for their continued support.

**Hazel Sparkes (Local Organiser)**

## March for Science

Prior to the March, the BCA Council adopted the following resolution:  
In accord with the mission and principles of the BCA, the Council of the BCA has voted to endorse the March for Science, which is taking place on April 22nd at over 500 locations around the world, including six cities in the UK.

The stated mission of the March for Science (<https://www.marchforscience.com>) is:

**The March for Science champions robustly funded and publicly communicated science as a pillar of human freedom and prosperity. We unite as a diverse, nonpartisan group to call for science that upholds the common good and for political leaders and policy makers to enact evidence based policies in the public interest.**

Marches were held in London, Bristol, Edinburgh, Cardiff, and Loughborough. London had 12,000 participants, Bristol had 2,000, Cardiff reports a small but enthusiastic contingent of 200.

**Marsha Nicholson** provided this information, and **Felipe Gonçalves** took the photos.

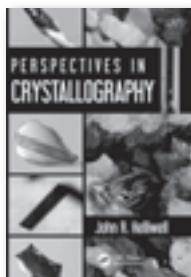


# Book Reviews

## Perspectives in Crystallography

John R. Helliwell

ISBN: 978-1-4987-3210-9



**FOR** readers of *Crystallography News* John Helliwell will be a well-known and well-respected person: BCA Spring Meeting chairman, ECA President and IUCr journal and *Crystallography Reviews* editor. His book immediately grabs one's attention with the colourful pictures of crystals on the cover. A hasty look inside suggests that this is a "Bitsa", assembled from fragments of

previous publications. A closer reading shows that the bits cohere. The first chapter describes some of the presentations to further the public understanding of crystallography given by the author to various audiences, including visitors to university open days, A-level chemistry students, audiences at a community centre lecture series, inmates of a prison and the sophisticated but non-specialist audience for a Royal Institution Discourse. While not many of us will have the latter opportunity, there are plenty of other ideas which we can follow.

The next section is historical, displaying milestones in the development of X-ray crystal structure determination. Its first chapter presents vignettes of some of the most important papers by W H and W L Bragg, while the emphasis of its second chapter is more on evaluations of the work in statements by the Braggs and other key players. The method is made clear by which the conundrum was overcome that we cannot know unit cell dimensions without knowing the wavelength of the radiation applied, but we cannot measure the wavelength of reflected X-rays without knowing the spacing of the reflecting planes. This format is not immune to duplication; for instance, the first page of the paper entitled "The Reflection of X-rays by Crystals. (I)" explaining how this was done appears on page 24 and again on page 39.

It is obvious that a book describing the evolution of crystal structure determination like this one must start with the Braggs and continue by honouring Kathleen Lonsdale, but which topics of modern crystallography should be covered? John Helliwell has played to his own strengths, which are in particularly exciting areas. His chapter 4, the longest one, summarises crystallographic use of synchrotron radiation (SR), where he was involved from its inception. While still a postgraduate student in the mid-1970s, he was asked by Dorothy Hodgkin for his opinion on some preliminary experiments. Soon he began a long involvement with the world's first dedicated SR X-ray source at Daresbury Laboratory and subsequently with the third-generation ESRF in Grenoble. As well as documenting the theory and practice underlying the impressive advances in

SR instrumentation, this chapter describes the meticulous administration required for the establishment of new facilities and also the Journal of Synchrotron Radiation, along with the management of sudden crises such as the cracking of a concrete floor in Grenoble! An inspiring theme was the collaboration of scientists from across Europe to make the ESRF a success, and the willingness of American and Japanese scientists to share best practice. Near the end of this chapter neutron Laue macromolecular crystallography and its payoff in the location of water molecules in proteins are described.

Chapter 5 sets out the related theme of predicting and verifying protonation states in proteins. Hydrogen atoms are often involved in protein function, but locating them with confidence typically requires both neutron diffraction data and ultra-high resolution X-ray data. Otherwise, predictions would be valuable. Since the environment can significantly modify the standard pK<sub>a</sub> values of amino acids, software packages have been written to predict their protonation state in proteins. Three such tools were evaluated on four proteins for which neutron and ultra-high-resolution X-ray data were available. They were generally reliable in predicting deprotonated residues but less reliable for protonated ones. The effect of changing pH on the residues of ribonuclease A was well predicted, but predictions for the crucial His92 residue in crustacyanin were inconclusive.

Chapter 6 continues the topic of β-crustacyanin, comprising two related protein molecules each complexing the highly conjugated carotenoid astaxanthin. Crustacyanins give the lobster carapace a blue/black colour which changes to orange/red when cooked. Heat-induced denaturation of the protein is expected to give the astaxanthin molecules more freedom and change their degree of conjugation. These findings were highlighted in publications ranging from *Scientific American* to the *Liverpool Daily Post*.

The remaining chapters are brief. Chapter 7 presents optimistic predictions for the future of structure determination, based upon technological advances in crystallography as well as spectroscopic and computational techniques. Chapter 8 outlines the contribution crystallography can make to sustainability, both scientifically by its essential role in the discovery of new drugs and new materials for energy storage and conversion, and more broadly by its contribution to education and its distinguished record of gender diversity and peaceful international cooperation.

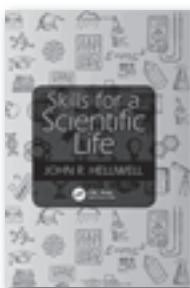
The brevity of the book (155 pages) restricts the breadth of coverage, but the comprehensive reference lists (165 references at the end of Chapter 4 alone) provide plenty of scope for further reading. Cost is kept down by reproducing most illustrations in black-and-white (as most of the original illustrations were anyway), but a 6-page section displays colour where it is most helpful (including the spectacular red gown worn by the Director of the Royal Institution!).

**Carl Schwalbe**

## Skills for a Scientific Life

John R. Helliwell

ISBN: 978-1-4987-6875-7



**SKILLS** for a Scientific Life is written as a 'how-to' manual for a successful scientific career and contains Professor Helliwell's engaging, personal accounts of his scientific life. He uses his experiences to provide practical guidance for all aspects of a scientist's career. Since Professor Helliwell's research area is crystallography, the book will be particularly relevant to the readers of

this magazine, but will also be of definite interest to any career scientist, particularly those employed in UK academia. One of the book's strengths is its central message that, to be a successful scientist today, one need not only have an excellent scientific mind, one must also engage with the administrative and communicative aspects of the job, as well as possess all of the other 'soft' skills that form part of a scientist's job, skills that in many cases have to be learnt.

The book is written in 34 succinct chapters, each focussed on specific aspects of a scientific career, with reference to examples from the author's experiences. Beginning with asking 'Am I suited to be a scientist', the subsequent chapters discuss research skills, reviewing others' work, being an educator, recognising the wider impact of your research, leadership roles, and scientific ethics. For any early- or mid-career scientists wondering about how they might progress up the academic ladder, this comprehensive guidance of what is important (and what is not!) will be of definite interest.

Becoming an academic inevitably means that the "only research" mindset of the Post-Doctoral Fellow must be put to one side and room must be made for the additional administrative and teaching responsibilities that are requirements of the role. The historical perspective on the introduction of increased professionalism into UK university teaching (e.g. peer-observation of teaching, quality assurance, progression panels for Doctoral students) is a useful reminder of how things have changed and that being a poor lecturer and an excellent scientist is no longer acceptable.

The sections on engagement with social media will also be relevant to Twitter-refuseniks and there is simple advice on who to follow and how often one should tweet; this theme is explored further in the discussions on effective communication with colleagues, as well as the public, in terms of explaining your research in language that is appropriate for the intended audience.

The book continues with reflections of practicing science at the highest level, as a head of Department or as leader of a learned society, before examining the issues of gender bias, and how Athena-Swan is underpinning efforts in the UK to improve prospects for women. Finally, there are sections on scientific ethics and how to drive scientific progress at a global level through collaborative links and at a national level by engaging with Governmental policy-making. The appendix contains 11 sections that are 'How to' guides for some of the

more generic workplace situations (e.g. keeping to a budget, delegation) that would be instructive across many professions.

The increasing number of STEM jobs in the UK<sup>[ref]</sup> is proof that there is a growing demand for excellent scientists with the necessary skillsets (scientific, administrative and communication skills). This clearly written and engaging book is full of sound, easily digestible advice (since it is borne out of the author's first-hand experiences) that cover all aspects of a scientific career, from selecting a degree course at University to arriving at the highest level, and would be a recommended and invaluable read for any aspirant scientific leaders in any science discipline.

Ref: *Nature* 542, 263 (09 February 2017)  
doi:10.1038/nj640-263c

**Edward Schwalbe**  
Northumbria University



## Puzzle Corner

WITH the IUCr Congress in Hyderabad coming up, identify the Indian scientists or scientific institutions from the clues. The first letters of their (sur)names should spell a macroscopic representation of an orthorhombic unit cell.

- With Einstein he can form a condensate.
- He turned protein crystallographers into plotters.
- Research institute founded in Kolkata in 1876; sounds a bit horticultural but does basic research.
- If you're a star, beware if you exceed his limit.
- He showed how the order of nucleotides controls protein synthesis.

# Obituaries

## Howard D. Flack (1943–2017)



**HOWARD** Flack died quite suddenly on Thursday 2 February 2017 from pneumonia contracted during treatment for recently diagnosed mesothelioma.

There can be no doubt that the direction of his life-long research interests was formed while he was studying under Kathleen Lonsdale at University College London. His PhD project, *Studies of disorder in anthrone and in mixed crystals of anthrone-anthraquinone*, exposed him to the need for a deep understanding of the diffraction process and its mathematical treatment. The introduction to his paper *Calculation of dimensions of ordered regions in triclinic and monoclinic pseudosymmetric crystals from the intensity of diffuse scattering* (Flack, 1970) reveals a train of thought that was to reemerge a decade later in his work on absolute structure determination, and his desire to provide a detailed mathematical explanation of physical processes.

After gaining his PhD, Howard moved to Cambridge (England) to work as Research Assistant in Surface Physics in The Cavendish Laboratory. It was at this time, 1971, that he started walking out with a Swiss girl, Evelyne, who had been sent to Cambridge by her employer in order to improve her English. Who better to teach her the Queen's English than Howard? It had been his intention to continue his studies in one of the Commonwealth countries, perhaps Australia or Canada, when by happy coincidence an opportunity opened to work with Erwin Parthé as Maître-assistant in the Laboratoire de Cristallographie at the University of Geneva, Switzerland. Howard moved to Switzerland in January 1972, and by the summer he and Evelyne were married. His arrival in Geneva coincided with a new start of crystallography in western Switzerland. Parthé's interdisciplinary Crystallography Laboratory was a new central facility serving the Faculty of Science of the university. A year later, an Institute of Crystallography was newly created at the University of Lausanne, while the Universities of Neuchâtel and Basel gradually developed structure determination services. Howard generously collaborated with all these start-ups and was involved in their success. For many years, the X-RAY76 program system (Stewart, 1976) was developed jointly at Geneva and Lausanne. Howard contributed code to X-RAY76 until its slow demise in the 1990s. Except for short periods spent elsewhere, he was to remain in Geneva until his retirement. He was employed as part of the technical staff, but his brilliance, wit, courage, and generous unselfish services to the Swiss and international crystallographic communities outshone his humble professional position.

From 1981 to 1990 he was secretary of the Swiss Society of Crystallography. His work with Parthé on highly absorbing

crystals of  $\text{SmAu}_6$  ( $\mu R = 5.9$ ) made him realize that the approximations made in the absorption corrections of North *et al.* (1968) and Kopfmann & Huber (1968) were inappropriate. The problem was resolved by representing the absorption profile as a Fourier series, an idea which has since been developed to use spherical harmonics. This and all subsequent non-analytical absorption corrections essentially reduce the sample to a sphere, which will have an effect which cannot be corrected for experimentally. Alternative suggestions for dealing with this residual error are given in the paper *Automatic absorption correction using intensity measurements from azimuthal scans* (Flack, 1974). The computations were implemented in the computer program CAMEL JOCKEY, an early example of his anarchic sense of humour. The absorption algorithm was extended and appeared as the program CAMEL JOCKEY WITH THREE HUMPS, also compatible with the X-RAY76 software system.

Howard continued to have a deep interest in the problems associated with obtaining the best quality experimental data, especially as a result of his growing interest in the determination of absolute structure by X-ray diffraction. Prior to Rogers' introduction of his  $\eta$  refinement, absolute structure estimation had depended on the careful examination of a small number of carefully measured reflections. Rogers' idea, related to earlier attempts to experimentally determine anomalous (resonant) scattering factors, introduced a refinable parameter into the main structure refinement (Rogers, 1981). Howard realized that the  $\eta$  parameter became singular midway between its extreme theoretical values, and that the problem could be better posed by regarding the sample as a twin containing  $x$  and  $1 - x$  twin fractions of the two enantiomers (with  $x$  a refinable parameter) (Flack, 1983) in an analogous way to his 1970 treatment of disorder. This elegant solution to the problem of absolute structure determination proved to be enormously popular, with the twin fraction  $x$  quickly being called the Flack parameter. Technical difficulties with its robust implementation were eventually resolved through practical experience and a reorganization of the algorithm (Parsons *et al.*, 2013).

Having opened Pandora's box, Howard was even more in demand as a speaker and authority on absolute structure determination. Since he was a good lecturer and he enjoyed direct interaction with other crystallographers, he accepted invitations as often as he could. He particularly enjoyed being with students and would take every opportunity to get them to talk about their own work. However, it sometimes seemed that he was disappointed that his work on chirality overshadowed other projects. He was saddened that concepts in the paper *On the definition and practical use of crystal-based azimuthal angles* (Schwarzenbach & Flack, 1989) were not widely adopted as a mechanism for sharing diffraction data. The paper *Merohedral twin interpretation spreadsheet, including command lines for SHELXL* (Flack & Wörle, 2013) seems to have attracted less attention than it deserves. As we noted earlier, Howard was always keen to provide a sound mathematical background to his ideas, and

some of this has been published in papers on the intensity statistics of Friedel pairs (e.g. Shmueli & Flack, 2009), though these papers too have not attracted a large audience.

Howard saw, very early on, the contribution modern computer-based communication systems could make to the dissemination of crystallography. His contributions to the digital publication of IUCr material, to the structured archiving of data and to the crystallographic community warrant their own description and are detailed at  
[http://www.iucr.org/people/crystallographers/flack\\_ep](http://www.iucr.org/people/crystallographers/flack_ep).

Howard's knowledge of the early crystallographic literature repeatedly led him to reinvestigate old problems. His very recent paper on the Patterson function (Flack, 2015) returns to the use of the resonant difference Patterson function, something he had briefly visited in *Practical applications of averages and differences of Friedel opposites* (Flack *et al.*, 2011). In that paper he wrote 'The Fourier transform of  $D$  has never been used in structure solution but a simulation by Woolfson (see International Tables for Crystallography, Vol. B, *Reciprocal Space*, ch. 2.3, pp. 235–263) confirms that it has interesting properties.' Naturally, Howard could not leave anything with 'interesting properties' alone for long.

Howard was in the middle of active collaborations when he fell ill, but he was determined not to let his condition interfere with his dreams. Just a few weeks before he died, he had drastically reorganized a draft manuscript and changed the prosaic title to '*HUG and SQUEEZE:*' etc. One could not help remembering the *CAMEL JOCKEY*, with or without the humps.

With Howard, we have not only lost an influential scientist and teacher, we have also lost a widely interested and cultured person. He was well read and familiar with, for example, Tristram Shandy as well as with the lore of Middle-earth. He loved music, opera and concerts. With Evelyne he assembled and restored an impressive collection of vintage toy trains and railway accessories produced by the British firm Hornby between 1920 and 1963. He was a good down-hill skier and horseback rider. And he was a wonderful companion with a fresh humour, funny and fair. He is survived by his wife Evelyne, his son Patrick and his daughter Christine.

## References

- Flack, H. D. (1970). *Philos. Trans. R. Soc. London Ser. A*, **266**, 575–582.  
Flack, H. D. (1974). *Acta Cryst.* **A30**, 569–573.  
Flack, H. D. (1983). *Acta Cryst.* **A39**, 876–881.  
Flack, H. D. (2015). *Z. Kristallogr.* **230**, 743–748.  
Flack, H. D., Sadki, M., Thompson, A. L. & Watkin, D. J. (2011). *Acta Cryst.* **A67**, 21–34.  
Flack, H. D. & Wörle, M. (2013). *J. Appl. Cryst.* **46**, 248–251.  
Kopfmann, G. & Huber, R. (1968). *Acta Cryst.* **A24**, 348–351.  
North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* **A24**, 351–359.  
Parsons, S., Flack, H. D. & Wagner, T. (2013). *Acta Cryst.* **B69**, 249–259.  
Rogers, D. (1981). *Acta Cryst.* **A37**, 734–741.  
Schwarzenbach, D. & Flack, H. D. (1989). *J. Appl. Cryst.* **22**, 601–605.  
Shmueli, U. & Flack, H. D. (2009). *Acta Cryst.* **A65**, 322–325.  
Stewart, J. M. (1976). Editor. *The X-ray System of Crystallographic Programs*. Technical Report TR-446. University of Maryland, USA.

**David Watkin (University of Oxford) and Dieter Schwarzenbach (École Polytechnique Fédérale de Lausanne)**

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**IN** October 1965 I started my PhD research in the laboratory of Kathleen Lonsdale at University College London as one of her last research students. Starting at the same time, and seated next to me was the then young **Howard Flack**, and we soon became good friends. Howard had studied Chemistry at Nottingham, if I recall correctly. He was assigned to work on diffuse scattering in crystals of anthrone and anthroquinone, whereas I studied mixed crystals of phenazine and phenazine-N-oxide, and it turned out that this showed diffuse scattering quite similar to that being studied by Howard. And so we worked closely together. It soon became apparent that Howard was much better in mathematics than I, whereas I was probably better at experiments. So we complemented each other well. One of the first tasks given to us by Kathleen Lonsdale was to use Beevers-Lipson strips as an exercise to plot the Fourier projection of hexamethyl benzene. Howard was much quicker off the mark than I to understand how to do that.



*The Chemistry Department at UCL in 1966. Howard can be seen 5th from the left in the middle row.*

We were very lucky in Kathleen Lonsdale's research group as we had for our own personal use a real computer. I think we may have been the only scientific research group anywhere with its own computer. This was a Ferranti Pegasus Mark II machine with 8K of store on a magnetic drum, and 5-hole paper tape. Programming was in machine code which was something that Howard mastered very quickly: it took me a lot longer to understand, but I could never match Howard's ability in this. This actual computer is now on show in the Science Museum in London (<https://blog.sciencemuseum.org.uk/the-pegaus-computer/>) and still has a coffee stain on the chair that I left there one night. The photo shows Howard and me working on the computer in 1966.

In 1966 Howard and I went together with Kathleen Lonsdale to Moscow to attend the IUCr Congress where she was standing in as President in place of J.D. Bernal, who was too ill to travel. She was able to pay our expenses in Russia because she had some money there from a book she had written on Quakers in Russia. I recall that we arrived at the wrong airport and had to wait for our host, Professor Zhdanov, to come across Moscow to meet us. It was at the height of the cold war, but we found everyone to be very friendly. On the ride into Moscow the interpreter, whose name was Valery Demidov, taught me and Howard several Russian swear words, and from that time most communications between Howard and myself started or ended with greetings using one of those swear words! Howard had a rather special sense of humour.



IUCr Congress Moscow 1966: In the main lecture hall of the Moscow State University. At the front, starting third along is Howard.



In front of the Pegasus computer examining some 5-hole paper tape (ca 1966).

In 1968 Howard and I published together six papers in *Phil. Trans. Roy. Soc.* and left University College. Howard had in his papers developed an early mathematical formulation for X-ray diffuse scattering. He then went to the Cavendish Laboratory, Cambridge and I to the Chemistry Department at Harvard. In September 1969 I moved to the Cavendish Laboratory, and although we were working in different parts of the Department we soon met up and even shared for a brief while a house together with a few other miscreants. I recall that the gas meter was fed continuously with the same coin simply by putting it into the top and collecting it again through a hole at the bottom. To keep the house warm, as it had no central heating, we simply put the oven on permanently in the kitchen and left the doors open so that the heat could permeate through the building! It was during that time that Howard discovered his future wife, a Swiss au pair called Evelyn and soon she moved into the house with Howard. Subsequently, Howard moved to Geneva and married Evelyn, and we only saw each other on occasion. He seemed to develop a French accent on speaking English remarkably quickly: given Howard's unusual sense of humour I was never sure if he was putting it on deliberately. We kept in contact and continued to discuss topics such as optical activity, chirality and the history of Louis Pasteur.

His death earlier this year came as a shock. He was a clever scientist and a good colleague. I shall miss him.

**Mike Glazer (University of Oxford)**

## Richard E. Marsh

(1922-2017)



### Remembering Caltech Crystallographer Richard Marsh

**RICHARD** Marsh (BS '43), senior research associate in chemistry, emeritus, at Caltech, passed away on January 3, 2017, at the age of 94.

Marsh, who went by the name Dick, was a crystallographer, and a colleague, mentor, and friend to generations of scientists. His career at Caltech started before World War II, spanned the golden age of structural chemistry led by Caltech's Linus Pauling, and continued to flourish into the 21st century. Crystallography is an experimental approach for determining in detail the locations of the atoms in a molecule by analyzing how X-rays are scattered from a crystalline sample of that compound.

"Dick was a legendary one-of-a-kind crystallographer who was recognized for his mastery of the field and his rigorous standards. He trained generations of students and postdocs and was widely respected as representing the heart and soul of crystallography," says Doug Rees, the Roscoe Gilkey Dickinson Professor of Chemistry and faculty director of the Molecular Observatory for Macromolecular Crystallography at Caltech.

Marsh was born in Jackson, Michigan, in 1922. He arrived at Caltech as a freshman in 1939, graduating with a degree in applied chemistry in 1943. "He would describe the required technical drawing course that he took with an enthusiasm that presaged his future talents in detailing molecular structure," says Rees.

Although Linus Pauling had established Caltech as a world center for crystallography around this time, Marsh's interest in this area did not begin then. In 1945, after Marsh was discharged from the US Navy in New Orleans, the home of his fiancée Helena Laterriere (whom he married in 1947), he started graduate school at Tulane University. He enrolled in the X-ray crystallography course at H. Sophie Newcomb College, the women's college of Tulane, as it was one of the few available classes with an opening. As reported in an issue of Caltech's *Engineering & Science* magazine, Marsh said the class changed his life, and that the instructor Rose Mooney inspired him to become a crystallographer. Tulane did not offer a PhD in chemistry, so after this introduction to crystallography, Marsh transferred to UCLA where he received his PhD in 1950 with James McCullough for crystallographic studies of organoselenium compounds, which are molecules with carbon-selenium bonds.

Marsh returned to Caltech in 1950 as a postdoctoral research fellow, working with Pauling on crystallography. He became a research associate in 1973, senior research associate in 1981, and senior research associate, emeritus, in 1990. Marsh was critically involved in many noteworthy structural developments, including work on hydrates, trimesic acid, protonated water clusters, intermetallic compounds, and the detailed geometry of amino acids and peptides. Marsh's structural study of a protein in silk called fibroin culminated in

the textbook model for a protein structural feature called the anti-parallel beta sheet. That research still resonates today for its implications in the architecture of amyloid fibril plaques associated with neurodegenerative diseases like Alzheimer's.

"Dick Marsh was an exceptionally talented crystallographer whose work had enormous impact on young and old investigators alike," says Harry Gray, Arnold O. Beckman Professor of Chemistry at Caltech. "I learned so much discussing structures with him. I knew that if he couldn't solve a structure, it couldn't be solved!"

A characteristic of Marsh's research was to carefully analyze the errors in a crystal structure determination. Rees recalls that Marsh was particularly upset about the most egregious cases of incorrect structure determinations, often due to erroneous assignments of the underlying arrangements of the constituent molecules in crystals. As Marsh noted in his crystallographic history: "I somehow take such errors personally: they should not happen in MY field of study."

From his office in the Beckman Institute at Caltech, Marsh continued surveying and correcting reported structures for the rest of his life. "The threat to other crystallographers of being publicly 'Marshed' for publishing a problematic structure undoubtedly contributed to increased scrutiny and care that prevented a number of incorrect crystal structures from ever being published," says Rees.

He served as president of the American Crystallographic Association in 1993, and was co-editor of *Acta Crystallographica* from 1964 to 1971. He was the first recipient in 2004 of the American Crystallographic Association's Kenneth N. Trueblood Award, given for exceptional achievement in computational or chemical crystallography.

Marsh was a research mentor to both students and young faculty. John Bercaw, Caltech's Centennial Professor of Chemistry, Emeritus, recalls approaching Marsh back in 1975 to help solve the structure of a key compound that cleanly generates hydrazine from molecular nitrogen. Bercaw had been informed that solving the compound's crystal structure was not possible. After Bercaw explained to Marsh the major importance of obtaining this crystal structure, Marsh immediately accepted the challenge and devised a method for solving the structure, allowing for further studies of the mechanism of hydrazine formation.



Richard Marsh celebrates Linus Pauling's 85th birthday at Caltech in 1986. From left to right: Brahma Sharma, Richard Marsh, Linus Pauling, Sten O. Samson, and Linus Pauling, Jr.

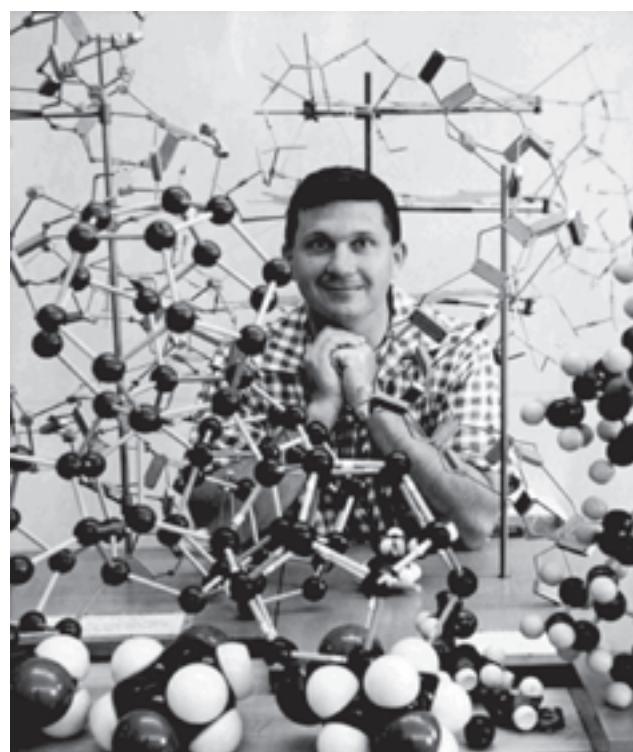
Credit: Caltech Archives

"Dick's inquisitiveness, integrity, compassion, and his intolerance of sloppy thinking and bureaucracy, epitomize the best traditions of Caltech, while highlighting the impact that one person can have on a field and generations of scientists," says Bercaw.

Marsh leaves behind his wife Helena; his four children Susan (Bill Winnie), Chip (Kay), Kirby (Bob Lauderback), and Stephen (Susan); 11 grandchildren and their spouses; and four great-grandchildren.

**Doug Rees**, edited by **Whitney Clavin**

*Reprinted by permission from Caltech*



Richard Marsh in 1960, surrounded by a molecular model.  
Credit: Caltech Archives



Richard Marsh with a student, Jenny Kung, in a lab at Caltech in 1974.  
Credit: Caltech Archives

# Meetings of interest

**FURTHER** information may be obtained from the websites given. If you have news of any meetings to add to the list, please send them to the Editor, c.h.schwalbe@hotmail.com . Assistance from the IUCr website and the *Journal of Applied Crystallography* is gratefully acknowledged.

## 4-9 June 2017

IMMW20: International Magnetic Measurement Workshop, Diamond Light Source.

<http://www.diamond.ac.uk/Home/Events/2017/IMMW20.html>

## 5-7 June 2017

New directions in porous crystalline materials: Faraday Discussion, Edinburgh.

<http://www.rsc.org/events/detail/20413/new-directions-in-porous-crystalline-materials-faraday-discussion>

## 5-7 June 2017

canSAS: Small Angle Scattering Workshop, San Francisco, CA, USA.

<https://sites.google.com/a/lbl.gov/cansas/home>

## 5-9 June 2017

International Workshop on Computational Nanotechnology, Windermere.

<http://iwcn2017.iopconfs.org/home>

## 5-9 June 2017

8th Workshop on Neutron Scattering Applications in Structural Biology, Oak Ridge, TN, USA.

<https://conference.sns.gov/event/66/>

## 5-9 June 2017

Session I - Fundamentals of X-ray Powder Diffraction. ICDD X-ray Diffraction Clinic, Newtown Square, PA, USA.

<http://www.icdd.com/education/xrd.htm>

## 6-9 June 2017

4th NovAliX Conference: Biophysics in Drug Discovery 2017, Strasbourg, France.

[http://www.idorganisation.com/v2/produits.php?langue=english&cle\\_menus=1238916384](http://www.idorganisation.com/v2/produits.php?langue=english&cle_menus=1238916384)

## 7-9 June 2017

Neutrons in Structural Biology, Grenoble, France.

<https://indico.ill.fr/indico/event/58/>

## 11-14 June 2017

1st RSC Anglo-Nordic Medicinal Chemistry Symposium, Snekkersten, Copenhagen, Denmark.

<http://www.maggichurchoousevents.co.uk/bmcs/>

## 11-22 June 2017

The Zurich School of Crystallography 2017: Bring Your Own Crystals, Zurich, Switzerland.

<http://www.chem.uzh.ch/linden/zsc/>

## 12-15 June 2017

Ultrafast X-ray Summer School (UXSS2017), Hamburg, Germany.

<https://conferences.cfel.de/uxss2017/>

## 12-16 June 2017

Session II - Advanced Methods in X-ray Powder Diffraction. ICDD X-ray Diffraction Clinic, Newtown Square, PA, USA.

<http://www.icdd.com/education/xrd.htm>

## 12-21 June 2017

Joint FEBS-EMBO Advanced Lecture Course: Molecular Architecture, Dynamics and Function of Biomembranes, Cargèse, Corsica, France.

<http://web.science.uu.nl/cargese2017/>

## 13-15 June 2017

Chemical Development & Scale-Up in the Fine Chemical and Pharmaceutical Industries, Edinburgh.

<https://www.scientificupdate.com/>

## 14-15 June 2017

Joint X-ray Diffraction and X-ray Fluorescence meeting, Leicester.

<http://www.crystallography.org.uk/>

## 19-23 June 2017

Mineral Fibres: Crystal Chemistry, Chemical-Physical Properties, Biological Interaction and Toxicity, Modena, Italy.

[http://emu2017.unimore.it/wp-content/uploads/2016/03/EMU2017\\_flyer.pdf](http://emu2017.unimore.it/wp-content/uploads/2016/03/EMU2017_flyer.pdf)

## 19-23 June 2017

5th EIROforum (ESI 2017). School of Instrumentation, Schenefeld, Germany.

<https://indico.cern.ch/event/588382/>

## 19-26 June 2017

10th annual CCP4 crystallographic school "From data collection to structure refinement and beyond", Argonne, IL, USA.

<http://www ccp4.ac.uk/schools/APS-2017/index.php>

## 24-25 June 2017

Crystal Growth and Assembly (Gordon Research Seminar), Biddeford, ME, USA.

<http://www.grc.org/programs.aspx?id=17340>

## 25-30 June 2017

Gordon Research Conference on Crystal Growth and Assembly, Biddeford, ME, USA.

<http://www.grc.org/programs.aspx?id=12674>

## 26-30 June 2017

EMBL-EBI Summer School in Bioinformatics, Hinxton, Cambridge.

<http://www.ebi.ac.uk/training/events/2017/summer-school-bioinformatics-0>

## 26-30 June 2017

ICTMS 2017: 3rd International Conference on Tomography of Materials and Structures, Lund, Sweden.

<http://ictms2017.lth.se/>

**27-29 June 2017**

LCF8. Eighth International Conference on Low Cycle Fatigue, Dresden, Germany.  
<http://www.lcf8.de/>

**27-30 June 2017**

48th BACG Annual Conference, Manchester.  
<http://www.bacg-2017.co.uk/23786?platform=hootsuite>

**27-30 June 2017**

MLZ Conference Neutrons for Health, Bad Reichenhall, Germany.  
<https://webapps.frm2.tum.de/indico/event/48/>

**1-8 July 2017**

4th Course of the Erice School: Neutron Science and Instrumentation, Erice, Sicily, Italy.  
<http://sons.uniroma2.it/ericeneutronschool/iv-course/>

**2-7 July 2017**

4th European Crystallographic School (ECS4), Warsaw, Poland.  
<http://ecs4.ecanews.org/>

**3-5 July 2017**

VHCF7. Seventh International Conference on Very High Cycle Fatigue, Dresden, Germany.  
<http://www.vhcf7.de/>

**3-6 July 2017**

Microscience Microscopy Congress 2017, Manchester.  
<http://www.mmc-series.org.uk/>

**3-7 July 2017**

7th FEZA Conference The ZEOLITES: Materials with Engineered Properties, Sofia, Bulgaria.  
<http://feza2017.org/>

**3-8 July 2017**

8th Workshop on Combined Analysis In XRD By Using MAUD Software, Caen, France.  
<http://maud.radiographema.eu/>

**4 July 2017**

Materials chemistry research and the economic health of the nation, Liverpool.  
<https://www.liverpool.ac.uk/events/series/?seriesid=381>

**4 July 2017**

Characterisation of Materials used in Nuclear Environments, London.  
<https://www.iopconferences.org/>

**6-7 July 2017**

Cryo-Electron Microscopy Symposium, Grenoble, France.  
<http://www.esrf.eu/cryo-em.fr>

**6-14 July 2017**

EMBO Practical Course: High-throughput protein production and crystallization, Harwell.  
<http://meetings.embo.org/event/17-protein-production>

**8-9 July 2017**

FEZA School, Sofia, Bulgaria.  
<http://feza2017.org/feza-school/>

**9-13 July 2017**

International Conference on Neutron Scattering 2017, Daejon, Republic of Korea.  
<http://www.icns2017.org/>

**10-12 July 2017**

UK Colloids 2017, Manchester.  
<http://constableandsmith.com/events/uk-colloids-2017>

**10-13 July 2017**

13th International Conference on Materials Chemistry (MC13), Liverpool.  
<http://www.rsc.org/events/detail/21273/13th-international-conference-on-materials-chemistry-mc13>

**12-14 July 2017**

The Francis Crick Electron Microscopy Opening Symposium, London.  
<http://www.rms.org.uk/discover-engage/event-calendar/crick-electron-microscopy-opening-symposium.html>

**13 July 2017**

FFEA Workshop, Leeds.  
[http://www.ccpem.ac.uk/training/leeds\\_em\\_md\\_2017/leads\\_em\\_md.php](http://www.ccpem.ac.uk/training/leeds_em_md_2017/leads_em_md.php)

**14 July 2017**

CCPBioSim-EM Workshop. Computation for Biomolecular Cryo-Electron Microscopy and Tomography, Leeds.  
[http://www.ccpem.ac.uk/training/leeds\\_em\\_md\\_2017/leads\\_em\\_md.php](http://www.ccpem.ac.uk/training/leeds_em_md_2017/leads_em_md.php)

**16-20 July 2017**

19th IUPAB Congress and 11th EBSA Congress, Edinburgh.  
<http://www.iupab2017.org/home>

**23-27 July 2017**

16th European Conference on Solid State Chemistry, Glasgow.  
<https://ecssc16.com/>

**23-28 July 2017**

AUC 2017 - The 23rd International AUC Workshop and Symposium, Glasgow.  
<http://auc2017.uthscsa.edu/>

**24-27 July 2017**

PS31.Protein Society's 31st Annual Symposium, Montreal, Canada.

<http://www.proteinsociety.org/page/annual-symposium>

**24-28 July 2017**

9th International Conference on Borate Glasses, Crystals and Melts and 2nd International Conference on Phosphate Glasses, Oxford.

<http://www.borate-phosphate.sgt.org/>

**26-28 July 2017**

CERMODEL - Modelling and Simulation Meet Innovation in Ceramics Technology, Trento, Italy.

<http://events.unitn.it/en/cermodel2017>

**26-28 July 2017**

Materials and Renewable Energy Conference, Hatfield.

<http://www.herts.ac.uk/mre/conference>

**30 July – 4 August 2017**

21st American Conference on Crystal Growth and Epitaxy (ACCGE-21) and 18th US Workshop on Organometallic Vapor Phase Epitaxy (OMVPE-18), Santa Fe, NM, USA.  
<http://www.crystalgrowth.org/Santa-Fe.html>

**31 July – 4 August 2017**

Denver X-ray Conference, Big Sky, MT, USA.  
<http://www.dxcicdd.com>

**6-10 August 2017**

Microscopy & Microanalysis (M&M2017), St Louis, MO, USA.  
<http://www.microscopy.org/MandM/2017/>

**6-10 August 2017**

X-ray Nanoimaging: Instruments and Methods III, San Diego, CA, USA.  
<http://spie.org/OPO/conferencedetails/x-ray-nanoimaging>

**7-17 August 2017**

Hydrogen School 2017, Berlin, Germany.  
[https://www.helmholtz-berlin.de/events/hydrogenschool/index\\_en.html](https://www.helmholtz-berlin.de/events/hydrogenschool/index_en.html)

**8-10 August 2017**

International Workshop on Topological Structures in Ferroic Materials, Leeds.  
<http://topo2017.iopconfs.org/home>

**14-15 August 2017**

International Workshop on Improving Data Quality in XAFS Spectroscopy, Diamond Light Source.  
<http://www.diamond.ac.uk/Home/Events/2017/Q2XAFS2017.html>

**17-20 August 2017**

Pharmaceutical Powder X-ray Diffraction Symposium, Hyderabad, India.  
<http://www.icdd.com/ppxrd/index.htm>

**20-26 August 2017**

2017 St Andrews CCP4 Protein Crystallography Summer School, St Andrews.  
<https://synergy.st-andrews.ac.uk/bsrc/>

**21-25 August 2017**

Microscopy Conference 2017, Lausanne, Switzerland.  
<http://www.mc2017.ch/>

**21-28 August 2017**

24th Congress of the International Union of Crystallography, Hyderabad, India.  
<http://www.iucr2017.org>

**28 August – 1 September 2017**

(IXS2017). 10th International Conference on Inelastic X-ray Scattering, DESY, Hamburg, Germany.  
<https://indico.desy.de/conferenceDisplay.py?confId=13621>

**30 August – 1 September 2017**

EMBO Conference: The Nucleosome: from Atoms to Genomes, EMBO, Heidelberg, Germany.  
<https://www.embl.de/training/events/2017/NUC17-01/>

**30 August – 4 September 2017**

International School on Fundamental Crystallography and Workshop on Structural Phase Transitions, Osisha, India.  
<http://www.iucr2017.org/wp-content/uploads/2016/09/School.pdf>

**3-6 September 2017**

7th Cambridge Symposium on Nucleic Acids Chemistry and Biology, Cambridge.  
<http://www.rsc.org/events/detail/23735/7th-cambridge-symposium-on-nucleic-acids-chemistry-and-biology>

**3-6 September 2017**

ISIC20. 20th International Symposium on Industrial Crystallography, Dublin, Ireland.  
<http://isic20.com/>

**3-6 September 2017**

AIC International Crystallography School (AICS2017), Pavia, Italy.  
<http://www.cristalografia.org/aicschool2017/eng/detail.asp?idn=2949>

**3-8 September 2017**

55th EHPRG Meeting: High Pressure Science and Technology, Poznan, Poland.  
<http://www.ehprg2017.org/>

**3-15 September 2017**

15th Oxford School on Neutron Scattering, Oxford.  
<http://www.oxfordneutronschool.org/>

**4-5 September 2017**

Advances in Quantum Transport in Low-Dimensional Systems, London.  
<http://aqt2017.iopconfs.org/home>

**4-15 September 2017**

JCNS Laboratory Course Neutron Scattering, Munich, Germany.  
[http://www.fz-juelich.de/jcns/EN/Leistungen/ConferencesAndWorkshops/LabCourse/\\_node.html](http://www.fz-juelich.de/jcns/EN/Leistungen/ConferencesAndWorkshops/LabCourse/_node.html)

**5-15 September 2017**

EMBO practical course on image processing for cryo-electron microscopy, London.  
<http://meetings.embo.org/event/17-cryo-em>

**11-15 September 2017**

EMBO Practical Course SAXS/SANS, Grenoble, France.  
<http://meetings.embo.org/event/17-small-angle-scattering>

**12 September 2017**

Swiss Society of Crystallography Annual Meeting, Geneva, Switzerland.  
<http://www.sgk-sscr.ch/en/geneva2017/>

**12-15 September 2017**

6th International caesar Conference. Overcoming Barriers: Atomic-resolution and beyond: advances in molecular electron microscopy, Bonn, Germany.  
<https://www.caesar.de/en/events/2017/6th-international-caesar-conference-overcoming-barriers.html>

**17-22 September 2017**

EUROMAT2017 Symposium: Materials Science with Synchrotron Radiation X-ray, Thessaloniki, Greece.  
<http://euromat2017.fems.eu/>

**19-21 September 2017**

Methods and applications in the frontier between MX and CryoEM, Barcelona, Spain.  
<http://www.sbu.csic.es/conference-mx-cryoem-bcn/>

**25-28 September 2017**

WIRMS 2017- Infrared Microscopy and Spectroscopy with Accelerator Based Sources Workshop, Oxford.  
<http://www.wirms2017.com/>

**26-27 September 2017**

SAXS Excites: The International SAXS Symposium 2017, Graz, Austria.  
<http://www.anton-paar.com/tu-graz/saxs-excites/>

**28-30 September 2017**

20th Heart of Europe Bio-Crystallography (HEC meeting), Wojanow Castle, Poland.  
<http://hec-20.iimcb.gov.pl/>

**2-6 October 2017**

Intermetallics Conference 2017, Bad Staffelstein, Germany.  
<http://www.intermetallics-conference.de>

**4-6 October 2017**

6th Joint Workshop on High Pressure, Planetary and Plasma Physics (HP4), Göttingen, Germany.  
[https://indico.desy.de/conferenceDisplay.py?  
confId=16402](https://indico.desy.de/conferenceDisplay.py?confId=16402)

**15-20 October 2017**

6th Accelerator Reliability Workshop. ARW 2017, Versailles, France.  
[http://www.synchrotron-  
soleil.fr/Workshops/2017/ARW-2017](http://www.synchrotron-soleil.fr/Workshops/2017/ARW-2017)

**16-19 October 2017**

25th International Conference on Materials and Technology, Portorož, Slovenia.  
<http://icmt25.com/en/>

**19-21 October 2017**

The 75th Annual Pittsburgh Diffraction Conference, Indiana, PA, USA.  
<http://www.pittdifsoc.org/conference.htm>

**23-27 October 2017**

Structural Bioinformatics, Hinxton, Cambridge.  
[http://www.ebi.ac.uk/training/events/2017/structural-  
bioinformatics-1](http://www.ebi.ac.uk/training/events/2017/structural-bioinformatics-1)

**28 October – 1 November 2017**

10th General Meeting of the International Proteolysis Society, Banff, Alberta, Canada.  
<http://www.ips2017.org/>

**29 October – 3 November 2017**

Advanced Topics in EM Structure Determination: Challenges and Opportunities, New York, NY, USA.  
<http://nramm.nysbc.org/participants-guide/>

**12-14 November 2017**

25th Protein Structure Determination in Industry Meeting, Cambridge.  
<http://www.psdi2017.org/25117>

**12-14 November 2017**

From Single- to Multiomics: Applications and Challenges in Data Integration, Heidelberg, Germany.  
<https://www.embo-embl-symposia.org/>

**16-17 November 2017**

EMBL Conference: Revolutions in Structural Biology: Celebrating the 100th Anniversary of Sir John Kendrew, Heidelberg, Germany.  
<https://www.embl.de/training/events/2017/JKS17-01>

**26 November – 1 December 2017**

2017 MRS Fall Meeting and Exhibit, Boston, MA, USA.  
<https://www.mrs.org/fall2017>





[www.iucr2017.org](http://www.iucr2017.org)

**24<sup>th</sup> Congress and General Assembly  
of the International Union of Crystallography  
Hyderabad International Convention Centre  
21 - 28 August 2017, Hyderabad, India**



### Plenary Lectures

- **Susumu Kitagawa** - Crystallography of dynamic structures and properties of porous coordination polymers / metal - organic frameworks
- **John Spence** - Crystallography with X-ray lasers
- **Giacomo Chiari** - Crystallography in art and cultural heritage

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